Understanding light-scattering particle discrimination through the eyes of machine learning

Patricio G. Piedra*, Christian Golbert, Yongle Pan, Aimable Kalume, and Gorden Videen

U.S. Army Research Laboratory, 2800 Powder Mill Rd, Adelphi, MD,USA

**Presenting author (patricio.g.piedracartagena.ctr@mail.mil)*

Discrimination of particles by light scattering is arguably one of the most important applications of light-scattering theory. However, although there exist accurate methods for discrimination of particles by inelastic scattering, discrimination by elastic scattering is much more challenging. The reason for this difficulty is that elastic scattering can vary substantially due to random particle rotations, shape, size, or refractive index, making it extremely difficult to simply minimize a light-scattering measurement against a model or a known measurement template. Recently, our team has demonstrated that deep learning can sort light-scattering signals of irregularly shaped particles very accurately (i.e., >92%) allowing for shape discrimination at a degree that would be virtually impossible in the past. However, although our algorithm was highly successful, we do not yet understand how deep learning acquires this very fine discrimination ability. In this work, we study the activation function of machine learning and try to bridge the gap of understanding between information brute-force processing and physics. We have applied a global average pooling layer connected to a dense-softmax layer in the final two layers of our newly developed architecture. The result is that we can obtain a weighted sum of convolutional activation maps from our final convolutional layer. Through this technique called class-activation mapping, we have mapped the angular dependence of activation of our light-scattering dataset and have highlighted which angular regions of light-scattering data are most activated for machine-learning discrimination. From these activation maps, we can explore some of the physics that are generalized by our machine-learning architecture. The results obtained in this work can aid in understanding which angles are the most efficient to place detectors in order to obtain fine discrimination by elastic light scattering.

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